Abstract

Title: **Homogeneous and Heterogeneous Reaction and Transformation of Hg and Trace Metals in Combustion Systems**

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OBJECTIVE

The objective of this program is to develop improved understanding of the transformations of mercury and other selected trace metals during coal combustion. As part of this effort, models will be developed for different trace metals that can be used to predict metal partitioning between vapor and condensed phase species. It is further expected that for the condensed phase species, these models will provide a dynamic means to predict the distribution between competing surface reactions and condensation as a function of post-combustion conditions. This would represent a significant advance over current models that are interpretive (i.e. that indicate whether condensation or surface reaction was dominant based on a fit to experimental data), and would provide a method for improving predictions of trace metal emissions and trace metal toxicity from a broad range of combustion systems.

The project consists of several experimental and model development tasks. These include:

- measurement of heterogeneous mercury oxidation reactions on solid surfaces including fly ash and synthetic fly ash surfaces to determine the effect of individual constituents (including carbon) in the ash, in a flame-based flow reactor in the presence of important post-flame radical species;

- determination of gas-solid reaction rates between As, Cd, Sb, and Se and reactive fly ash constituents (i.e. calcium oxide and iron oxide) as a function of trace metal concentration and gas temperature to obtain fundamental parameters needed for modeling metal partitioning;

- measurement of selected trace metal reactions in the flow reactor in the presence of contaminants such as NOx and SO_2;

- further development of a dynamic model that predicts partitioning by calculating competing rates of condensation and surface reaction for each metal, and thus incorporates boiler temperature profile, fly ash parameters, and gas phase chemistry.

Regulations to reduce the emissions of mercury from coal-fired power plants were recently announced by EPA. Initial experimental efforts will therefore focus on the chemistry of mercury, in an effort to provide timely data and models that can be used in the development of control strategies. Later stages of the program will focus on additional trace metals present in coal.

ACCOMPLISHMENTS TO DATE

Activity for the past year has centered on four areas: calculating equilibrium concentrations for trace metal compounds, characterizing synthetic fly ash, completing a literature search for available data on metal compound vapor pressures and relevant reaction rate constants, and developing a model which incorporates condensation and surface reaction as processes which add trace metals to particulate matter. The results from the equilibrium concentration calculations provided a basis for identifying compounds expected under a range of post-combustion conditions, to be used in selecting pertinent compounds for subsequent experiments. The synthetic fly ash characterization included scanning electron microscopy (SEM) and cascade impaction for particle size and BET-N_2 adsorption to determine particle surface area. These data will be useful when analyzing results from reaction and mass transfer rate experiments.

The completion of the literature search for vapor pressures and reaction rate constants has identified the reaction rates and mass transfer rates needed from planned laboratory experiments. Having set up the initial framework for the model, the focus of the project will now turn to collecting experimental data and verifying data gathered using the model calculations.

In the coming months, it is expected that activity will include initiation of experiments to study the interaction of trace metal compounds with different combinations of synthetic fly ash materials, and conducting initial experiments using flame gases.

FUTURE WORK

Work conducted during the next year of the project is expected to include experiments using aerosolized fly ash for comparison with fixed bed reactor experiments, and extraction of reaction rate constants for mercury oxidation reactions. Initial fixed bed experiments will be completed for other trace metals including As, Cd, Sb, and Se, and extraction of heterogeneous and gas-solid reaction rate parameters for these metals under post-combustion conditions.

PAPERS, PATENTS, PRESENTATIONS, STUDENTS SUPPORTED

There are no publications, patents, or presentations at this time.

This project is supporting Ms. Clara Smith, a full-time Ph.D. student in the Thayer School of Engineering at Dartmouth College.

Procedures for Submitting: The preferred format for submission is Microsoft Word or a PDF file that should be emailed to **Karen.lockhart@sa.netl.doe.gov.**